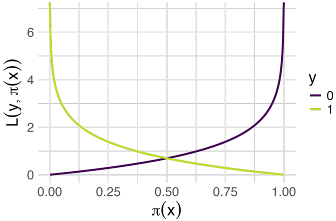
Introduction to Machine Learning

Advanced Risk Minimization
Proper Scoring Rules

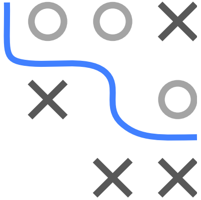


Learning goals

- Scoring rules on prob. predictions
- First order condition of SRs
- Log loss and Brier are strictly proper
- L1 on probs is not
- 0/1 is proper but not strict

PROB. PREDS / SCORING RULES

Gneiting and Raftery 2007



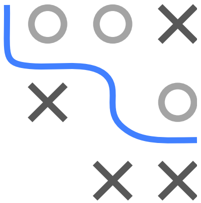
- Is specific loss $L\left(y, \pi(\mathbf{x})\right)$ on a prob. classifier "reasonable"?
- Assume binary classification with $y \in \{0, 1\}$
- Loss can already be called scoring rule, but we also now take expectation over y
- Scoring rule compares predictive vs. label distrib:

$$S(Q, P) = \mathbb{E}_{y \sim Q}[L(Q, P)]$$

- Simply expected loss, now we write P for $\pi(\mathbf{x})$
- We have looked at this before
- As we have seen in the beginning of this chapter:
  Can do this unconditionally or conditionally, all the same anyway
- Minimizing the above asks then for the risk minimizer!

PROPER SCORING RULE

Gneiting and Raftery 2007



- SR is **proper** if true label distrib Q is among the optimal solutions, when we maximize $S(Q, P)$ in the 2nd argument (for a given Q)

$$S(Q, Q) \leq S(Q, P) \text{ for all } P, Q$$

- Translation (now for conditional):
$\mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}})$ is **among the solutions** for the RM:

$$\eta(\tilde{\mathbf{x}}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}}) \in \pi^*(\tilde{\mathbf{x}})$$

- NB: We were never precise before that the RM as “argmin” is a set!
- S is **strictly proper** when equality holds iff $P = Q$
- Translation (now for conditional):
$\mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}})$ is unique RM!

$$\pi^*(\tilde{\mathbf{x}}) = \eta(\tilde{\mathbf{x}}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \tilde{\mathbf{x}})$$

- (Strictly) proper SR ensure optimization pushes solution $\pi(\mathbf{x})$ to Q

L1 LOSS IS NOT PROPER

- Let's look at it unconditionally, so we don't always have to write x
- Binary targets $y \sim \text{Bern}(\eta)$
- For any binary prob. loss L:

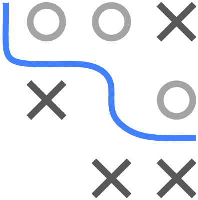
$$\mathbb{E}_y[L(y, \pi)] = \eta \cdot L(1, \pi) + (1 - \eta) \cdot L(0, \pi)$$

- Let's check L1 loss $L(y, \pi) = |y - \pi|$

$$\mathbb{E}_y[L(y, \pi)] = \eta|1 - \pi| + (1 - \eta)\pi = \eta + \pi(1 - 2\eta)$$

- Linear in π, but with box constraints
- For $\eta > 0.5$: $\pi^* = 1$
- For $\eta < 0.5$: $\pi^* = 0$
- So π^* usually not the same as η
- True η is worse than RM π^*, so L1 not proper SR

0/1 LOSS IS PROPER – BUT NOT STRICT



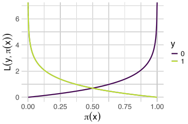
- **0/1 loss** $L(y, \pi) = \mathbb{1}_{\{y \neq h_\pi\}}$ using hard labeler $h_\pi = \mathbb{1}_{\{\pi \geq 0.5\}}$
- Expected loss:

$$\begin{aligned} \mathbb{E}_y[(y, \pi)] &= \eta \cdot L(1, \pi) + (1 - \eta) \cdot L(0, \pi) \\ &= \begin{cases} \eta & \text{if } h_\pi = 0 \\ 1 - \eta & \text{if } h_\pi = 1 \end{cases} \end{aligned}$$

- So expected loss only takes 2 values
- For $\eta \geq 0.5$, minimal if $h_\pi = 1$
  $\rightarrow$ any $\pi \in [0.5, 1]$ minimizes
- For $\eta < 0.5$ expected loss is minimal if $h_\pi = 0$
  $\rightarrow$ any $\pi \in [0, 0.5)$ minimizes
- True η among solutions $\rightarrow$ proper
- True η is not unique minimizer $\rightarrow$ not strictly proper

DISCOVER PROPER SCORING RULES

- How define L such that $\mathbb{E}_y[L(y, \pi)]$ is minimized at $\pi^* = \eta$?
- Assume symmetry: $L(1, \pi) = L(\pi)$ and $L(0, \pi) = L(1 - \pi)$
- Remember that when we plotted such losses, we usually had 2 curves, symmetric at $\pi = 0.5$?



- Then, with $\eta = \mathbb{P}(y = 1)$

$$\mathbb{E}_y[L(y, \pi)] = \eta \cdot L(\pi) + (1 - \eta) \cdot L(1 - \pi)$$

- First-order condition: Set $L'(\pi) = 0$, and $\pi = \eta$ at minimum

$$\eta \cdot L'(\eta) \stackrel{!}{=} (1 - \eta) \cdot L'(1 - \eta)$$

LOG LOSS / BRIER ARE STRICTLY PROPER

- First-order condition:

$$\eta \cdot L'(\eta) \stackrel{!}{=} (1-\eta) \cdot L'(1-\eta)$$

- One solution is $L'(\eta) = -1/\eta$
- Antiderivative is $L(\eta) = -\log(\eta)$
- Remember: $L(1, \pi) = L(\pi)$ and $L(0, \pi) = L(1-\pi)$
- This is **log loss**

$$L(y, \pi) = -y \cdot \log(\pi) - (1-y) \cdot \log(1-\pi)$$

- Second solution is $L'(\eta) = -2(1-\eta)$
- Antiderivative $L(\eta) = (1-\eta)^2$
- So **Brier score**

$$L(y, \pi) = (y-\pi)^2$$

- Both strictly proper (check 2nd derivative for strict convexity)

OUTLOOK

- Usually SRs are maximimized, I adapted notation a bit here for us, to get a direct connection ERM
- Was easier to talk about binary classification here, but proper SRs are defined in general
- There are other proper SRs, like “generalized entropy score” or ”continuous ranked probability score”
- We only scratched surface of theory
- If you want to know more: start by reading the Gneiting paper